Correlations in the high-energy photoeffect

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We examine correlations in high-energy photoeffect, utilizing a perturbative treatment of the effects beyond the independent particle approximation (IPA) in the high-energy photoionization of states with arbitrary values of the angular momenta ℓ. The dominant mechanism of IPA breaking is discussed. The dependence of IPA breaking contributions on the parameters $1/Z$ and αZ is analyzed. In the general case the amplitude is expressed as a linear combination of IPA amplitudes. The development of precise experiments, together with the demonstration that there is substantial cancellation among the nonrelativistic partial correlations amplitudes in many cases, particularly for ground-state atoms, makes a relativistic approach to the problem desirable, even at relatively low values of photon energy.

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We discuss the role of correlations in high-energy photoeffect. It was found in Ref. [1] that there is a large discrepancy between the experimental results and the independent particle approximation (IPA) calculations of L-shell ionization of neon by photons with energies of about 1 keV. It was shown in the same paper [1] that the discrepancy can be removed by inclusion of the interchannel correlations between $2p$ and $2s$ electrons, which goes beyond the IPA. Later [2] it was shown that in the case of angular distribution parameters at higher, but still nonrelativistic, energies correlations with the K shell cancel those inside the L shell to a large extent. A similar situation occurs for nitrogen [2]. There has been no relativistic analysis until now, while the use of a nonrelativistic asymptotic analysis could be questioned.

We investigate the contributions beyond the IPA to the cross sections for high-energy photoionization of states with arbitrary orbital momenta ℓ. We limit ourselves to the case of not very heavy atoms $(\alpha Z)^2 \ll 1$, with $\alpha = \frac{1}{137}$ being the fine-structure constant. Using a perturbative approach [3], we obtain the expression for the amplitudes of ionization of the states of any angular momenta ℓ as a linear combination of IPA amplitudes for this process. We consider both nonrelativistic and relativistic formulations, using relativistic notations for generality, but giving also the nonrelativistic reduction of the formulation. Our analysis is focused on the limiting cases of high, but still nonrelativistic, energies and of ultrarelativistic energies.

Within our approach we find that, at sufficiently high nonrelativistic energies, the nonrelativistic correlations in photoionization of a neutral atom in its ground state largely cancel, so that the actual importance of correlations requires a determination of relativistic correlations. We show that these cancellations, mentioned in the first paragraph as observed in angular distributions, are occurring in the matrix elements, and so they pertain to all observables. We show also that there is a general tendency toward such cancellations in other cases. Considering ionization of relativistic electrons, we focus on the ultrarelativistic case, showing how the correlations change the dependence on the parameter αZ.

By *high energy* we mean the photon energies ω strongly exceeding the ionization potentials $I_{n\ell}$ of the ionized $n\ell$ subshells, i.e.,

$$\omega \gg I_{n\ell}. \tag{1}$$

This means that the momentum of the outgoing electron p is much greater than the average momentum in the bound state $\tau_{n\ell} = (2mI_{n\ell})^{1/2}$, i.e.,

$$p \gg \tau_{n\ell} \tag{2}$$

(we assume the system of units with $\hbar = c = 1$).

At first glance the correlations caused by the final-state interactions (FSIs) of the ionized electron with the bound electrons of the residual ion are of the same order as the perturbative contribution of this interaction to the final-state wave function, i.e., of the order of the Sommerfeld parameter of this interaction,

$$\xi = \frac{\alpha E}{p}, \tag{3}$$

with p the momentum and $E = (p^2 + m^2)^{1/2}$ the total energy of the outgoing electron. At high energies (1) the value of ξ is small. In the nonrelativistic limit $\xi = m\alpha/p$, and thus $\xi^2 = 13.6\ \text{eV}/\varepsilon$ with $\varepsilon = p^2/2m$ being the nonrelativistic energy of the outgoing electron. At relativistic energies $\xi \sim \alpha$ and the correlation correction would seem to be as small as the radiative corrections, less than one percent. However, there is a mechanism, noted in Ref. [1], which enhances these correlations, as we now describe.

To estimate the magnitude of the correlation effects it is important for us to trace the dependence of the amplitudes on the momentum

$$\mathbf{q} = \mathbf{p} - \mathbf{k} \tag{4}$$

transferred to the nucleus ($\mathbf{p}$ and $\mathbf{k}$ are the three-dimensional momenta of the outgoing electron and of the photon, respectively). For large energies (1) one finds $q = |\mathbf{q}|$ to be much greater than the binding electron momentum $\tau_{n\ell}$, i.e.,

$$q \gg \tau_{n\ell}. \tag{5}$$

In the nonrelativistic limit $k = |\mathbf{k}| \ll p$, and up to the terms $I_{n\ell}/\omega$ and ω/m we can put $q^2 = 2m\omega$. In the general case $q > q_{min}$, with

$$q_{min} = (2m\omega + \omega^2)^{1/2} - \omega, \quad (6)$$

the minimum kinematically allowed value. In the ultrarelativistic limit $\omega \gg m$ one finds that $q_{min}=m$ up to the terms m/ω [4].

Once the large momentum q is transferred to the nucleus in the photoionization process, the amplitude is determined by the behavior of the wave function at small distances from the nucleus $\sim 1/q \ll \tau_{n\ell}^{-1}$. In the lowest order of the expansion in powers of $(\alpha Z)^2$ the wave function is proportional to $(\tau_{n\ell} r)^\ell$ at these distances. The factor $\tau_{n\ell}$ comes from normalization of the bound-state wave function. Hence the amplitude of ionization of an $n\ell$ state is $(\tau_{n\ell}/q)^\ell$ times smaller than that of ionization of an ns state. However, this quenching can be avoided if the photon interacts directly with any of the s states. The ionized s-state electron can then push an electron with orbital momentum ℓ into the hole in the s state which was created by the photon. This interaction takes place at distances of the order of the size of the bound states involved, as we shall see. The electron transfer amplitude contains one factor ξ, defined by Eq. (3), but it multiplies an s state IPA amplitude rather than the amplitude of ionization of the state with orbital momentum ℓ.

This mechanism, suggested in Ref. [1] to explain $2p$ photoionization of Ne, is the main IPA breaking mechanism in photoionization for high nonrelativistic energies of the outgoing electrons. The case of larger $\ell > 1$ was considered in Ref. [5]. Detailed calculations were carried out in Ref. [6]. In the nonrelativistic case the mechanism changes the asymptotic behavior of the cross sections from the IPA behavior $\sigma_{n\ell}^0 \sim \omega^{-7/2-\ell}$ [4] to $\sigma_{n\ell} \sim \omega^{-9/2}$ for all $\ell \geq 1$. We are labeling by ℓ the part of the multiconfiguration ground-state wave function which has ℓ state character. Thus for $\ell \geq 2$ the IPA breaking effects change the energy dependence of the cross section at high nonrelativistic energy. For $\ell = 1$ the energy dependence is not changed by the mechanism, while its asymptotic coefficient is. We note that there are further complexities in the energy dependence if one considers also the satellite lines [7].

In the relativistic case, inclusion of correlation effects changes the amplitude by terms of order $\xi q_{min}/\tau_{n\ell}$. The energy behavior of the cross sections is more complicated due to the dependence on the parameter ω/m. In the ultrarelativistic limit $E \gg m$ the energy dependence of all the photoionization cross sections is the same, while the correlations change the dependence on the parameter αZ.

The mechanism [1] is quite general, and it works at all photon energies greatly exceeding the binding energies of the electrons participating in the process.

This paper is organized as follows. In Sec. II we present the general high-energy formulation of the matrix elements and cross sections. The problem of slow convergence to the high-energy nonrelativistic limit is discussed in Sec. III, resolved by showing that the slowly convergent terms form a known factor, which is common for all photoionization amplitudes, and which thus cancels in the ratios. The asymptotic nonrelativistic results and the nature of the cancellation of the partial contributions (depending on atomic configuration) are considered in Sec. IV. Discussion of the relativistic case and estimation of asymptotic correlation effects is given in Sec. V.

A perturbative expression for the photoionization amplitudes, also valid in the relativistic region, can be obtained with the perturbative treatment of FSI worked out in Ref. [3]. Here we want to calculate the matrix elements and cross sections for asymptotic values of ω, which are much larger than all the binding energies. Since the largest binding energies are those in the K shell, where they can be estimated by the hydrogenlike formula $I_{10}=m(\alpha Z)^2/2$, the condition $\omega \gg I_{10}$ is equivalent to

$$\xi_Z^2 \ll 1, \quad (7)$$

with $\xi_Z = \xi Z$ being the Sommerfeld parameter of interaction between the outgoing electron and the nucleus. The corresponding equation for the amplitude has a simple form in the lowest order of expansion in powers of ξ_Z^2. In this limit we can neglect all interactions of the outgoing electron after it has caused transitions in the atomic shell.

In this approximation it is possible, even in the relativistic case, to work with the amplitudes F_i for ionization of a state with quantum numbers $i=n,\ell,\ell_z$, which can be represented as a linear combination of IPA amplitudes F_j^0 of ionization of atomic states j with the quantum numbers $j=n',0,0$,

$$F_i = F_i^0 + \sum_j F_j^0 \Lambda_{j,i}, \quad (8)$$

with Λ describing the transitions in the electronic shell caused by the outgoing electron. Here we have used the general expression obtained in Ref. [3], neglecting the terms which go beyond the asymptotics in our particular case.

Since the charge Z is not too large and $(\alpha Z)^2 \ll 1$, the averaged velocities of the bound electrons $(\alpha Z/n)^2 \ll 1$. Thus the electrons in the states i and j can be described by nonrelativistic functions. Then, the interaction v between the outgoing electron and the atomic shell, which causes transitions in the latter, is just the static Coulomb field (we neglect its possible modification by the other electrons). Note that it does not depend on the spin variables. Hence following Ref. [3] we can write

$$\Lambda_{j,i} = \int \frac{d^3f}{(2\pi)^3} \frac{2E}{f^2 + 2(\mathbf{p}\cdot\mathbf{f}) + 2E\delta_{j,i}} V_{j,i}(f). \quad (9)$$

Here $\delta_{j,i}=I_j - I_i$ is the difference between the binding energies $(I_{i,j}>0)$, while

$$V_{j,i}(f) = v(f)\langle j|e^{i(\mathbf{f}\cdot\mathbf{r})}|i\rangle. \quad (10)$$

Here $\langle i|$ and $\langle j|$ are the single-electron states in the atom. The interaction $V(f)$ can be treated as the perturbation which is suffered by the wave function of the outgoing electron. In Eq. (10) $v(f)$ is the Fourier transform of the interaction between the outgoing and the bound electrons. Following the analysis presented above we can put $v(f)=4\pi\alpha/f^2$.

In further estimations we assume that the sizes of the bound states i and j are of the same order of magnitude (the effect is quenched if these values differ strongly), and thus $\tau_{n\ell} \sim \tau_{n'0}$. The matrix element in Eq. (10) is determined at distances r of the order of the size of the bound states. Thus the integral over f on the right-hand side of Eq. (9) is determined at small $f \sim \tau_{n\ell}$. This enables us to extract the factor ξ in a natural way as

$$\Lambda_{j,i} = i\xi S_{j,i}. \tag{11}$$

The matrix elements $S_{j,i}$ describe the transfer of an electron from the states i to fill the hole in the state j of the positive ion. Taking the direction of the outgoing electron momentum as the axis of quantization of angular momentum, we find that the mechanism works only for i states with $\ell_z=0$. Note that Eqs. (8)–(10) are valid for all energies $\omega \gg m(\alpha Z)^2/2$. In the asymptotics all s states j contribute. Since $v(f)$ does not depend on the spin variables, the electrons in the states $\langle i|$ and $\langle j|$ should have the same spin projection, thus forming a spin triplet state. In the nonrelativistic limit we must put $E=m$ in Eq. (3). In the ultrarelativistic limit we must put $E=\omega$ and $\xi=\alpha$.

Now Eq. (8) can be written in the whole high-energy region as

$$F_i = F_i^0 + i\xi \sum_j F_j^0 S_{j,i}. \tag{12}$$

Here the factor ξ comes from the perturbative treatment of the FSI matrix element. In $S_{j,i}$ the angular dependence is separated out in a straightforward way, and the dependence on the IPA wave functions enters through the overlaps of the radial parts $\langle \psi_{n'0}^{(r)} | \psi_{n\ell}^{(r)} \rangle$. The calculation of Ref. [3] gives

$$S_{j,i} = \langle j | ln(1-t) | i \rangle, \tag{13}$$

where $t=(\mathbf{p}\cdot\mathbf{r})/pr$ and $\mathbf{p}$ is the momentum of the outgoing electron.

Squaring the amplitude, from Eq. (8) we have

$$|F_i|^2 - |F_i^0|^2 = 2\,\mathrm{Re}\left(i\xi \sum_j F_j^0 S_{j,i} F_i^0 \right) + \xi^2 \left| \sum_j S_{j,i} F_j^0 \right|^2. \tag{14}$$

The cross sections can be obtained by integration over the angular variables. This approach in our case includes contributions through terms of order ξ^2. In the general case, with arbitrary values for the orbital momenta of the states i and j, terms beyond Eq. (8) which involve two interactions in the final state also provide contributions of the order ξ^2. The corresponding equations are presented in Ref. [3]. However, in our case with different angular momenta, one of them being zero, such terms only contribute beyond the leading asymptotic behavior.

While the recent experiments on ionization of the outer shells of neon [1] and of argon [8] by photons with energies of about 1 keV demonstrated deviations from the IPA predictions, a nonrelativistic account of correlations between the outer electrons [1,6,8], neglecting correlations with more inner shells, improved the situation. However, to obtain quantitative results at higher energies one will need to sum over j in Eqs. (12) and (14). Calculations for higher energies of about 10 keV for the outer shells of N and Ne [2] demonstrated in a particular case the interplay of correlations within the L shell and with the electrons of the K shell (now important), with strong cancellations for angular distribution parameters. But in fact the general features of the sum have not yet been discussed for the nonrelativistic case. Therefore let us now discuss the nonrelativistic sum over j, to establish the expected size of correlations at high energies, where all correlation contributions are asymptotic.

It was at first not clear if there is a region where the nonrelativistic asymptotic analysis works, since the cross sections converge to this limit very slowly. The problem and its remedy can be understood [9–11]. Indeed, corrections to the asymptotic results are of the order $1/p$ with rather large numerical coefficients. The interactions of the outgoing electron with the residual ion can be expressed in terms of two parameters, $\xi_Z^2 = \xi^2 Z^2$ [ξ is given by Eq. (3)], and $\pi\xi_Z$. The terms which depend on $\pi\xi_Z$ come from the interaction between the outgoing electron and the nucleus at small distances of the order $1/p$, and it is these terms which converge slowly. The terms which depend on ξ_Z^2 come from the interactions between the electron and the nucleus at distances of the order of the size of the atom. The dependence on $\pi\xi_Z$ can be extracted explicitly as a "Stobbe factor" (SF) [10,11], which is a certain function of the energy of the outgoing electron. In leading order the factor is the same for the ionization amplitudes of all the bound states. This was demonstrated already in Ref. [12] for the hydrogenlike case, but it is much more general. Being a function of the energy of the outgoing electron, the Stobbe factor has dependence on the characteristics of the bound states (i.e., on the binding energies) beyond the leading asymptotic Stobbe term.

It was shown in Ref. [10] that due to the SF the cross section ratios $R_{n\ell}(\omega) = \sigma_{n0}(\omega)/\sigma_{n\ell}(\omega)$ converge to the asymptotic limit much faster than the cross sections themselves. The Stobbe factor is present in all photoionization cross sections, and it is primarily responsible for the slow convergence. This was confirmed in numerical calculations in the Hartree-Fock (HF) approximation, showing that one can use the $1/\omega$ expansion of the cross-section ratios at nonrelativistic energies.

Note that, in the approach described in the previous section, the SF is present in the amplitudes beyond the IPA as well. In Ref. [6] the IPA breaking amplitudes were obtained as linear combinations of IPA amplitudes, each of them having the SF. The coefficients of these combinations are given in terms of overlap matrix elements, which are determined at large distances of the order of the size of the atom. On the other hand, the SF is determined at small distances of the order $1/p$ [3,11]. Thus the IPA breaking amplitudes also contain the SF [6,10], making it possible to carry out the nonrelativistic asymptotic analysis beyond the IPA.

The SF can be extracted in the relativistic case as well. Its explicit leading term

$$S(E) = \exp(-\pi\xi Z)$$

is valid in the whole high-energy region. In the high-energy nonrelativistic limit we find $S(E)=1$, while in the ultrarelativistic limit $S(E)=\exp(-\pi\alpha Z)$.

In the asymptotic nonrelativistic case the photon momentum $\mathbf{k}$ is much smaller than the momentum $\mathbf{p}$ of the outgoing electron. In the lowest order of the expansion in powers of k/p the angular dependence of the IPA amplitudes, on the right-hand side (rhs) of Eq. (14), becomes simple. This allows us to carry out the angular integration of Eq. (14), obtaining an equation for the IPA breaking effects in the IPA cross sections σ_i^0 [6],

$$\sigma_i - \sigma_i^0 = 2\xi \sum_j S_{i,j}(\sigma_j^0 \sigma_i^0)^{1/2} + \xi^2 \left(\sum_j S_{i,j}(\sigma_j^0)^{1/2} \right)^2. \quad (15)$$

In Refs. [5,6] this equation was used for the calculation of IPA breaking effects in the nonrelativistic case. The results are especially simple for the asymptotic case [5,6]. However, somewhat more complicated expressions, which are valid beyond the asymptotic region, were obtained in Ref. [6] for the cases studied in Refs. [1,8]. The results obtained in Ref. [6] either eliminated or much diminished the difference between the experimental data for L and M shell ionization and the IPA calculations. As expected [13], the perturbative approach and a numerical random-phase approximation calculation [6] gave similar results. It was also argued in Ref. [6] that at the energies considered in Refs. [1,8] the correlations with the K shell give a minor contribution. However, it was shown in Ref. [2] that at larger energies correlations inside the L shell, and between L and K shells, in N and Ne cancel each other to a large extent, at least for angular distribution parameters.

We here report that the tendency for such cancellation is a general feature of the asymptotic matrix elements for neutral atoms in their ground states.

For the case of $\ell=1$, taking account of IPA breaking effects does not alter the linear law for the ratio, which we write as $R_{n1}=r_n\omega$. However, IPA breaking effects change the IPA value $r_n=r_n^0$ to

$$r_n = \frac{r_n^0}{1+\kappa}; \quad \kappa = \sum_{n'} \kappa_{n'} + \sum_{n' \neq n''} \eta_{n',n''}. \quad (16)$$

Here $\kappa_{n'}$ are the sums of the partial contribution of an s electron with principal number n' to the first term of the rhs of Eq. (15), and of the contributions with $n'=n''$ of the second term of the rhs of Eq. (15), while $\eta_{n',n''}$ are cross terms involving products of the contributions of s electrons with principal quantum numbers n' and n'', in the second term on the rhs of Eq. (15).

We use Eq. (15) to analyze the interplay of the partial contributions in the nonrelativistic asymptotics. Using the data on photoionization cross sections [14], we find strong cancellations for the cases considered in Ref. [2]. Our calculations were carried out for ionization of $2p$ states by a photon of energy $\omega=10$ keV. For nitrogen we found $\kappa_1=-0.29$, $\kappa_2=0.44$, $\eta_{1,2}=-0.23$, resulting in $\kappa=-0.08$. We found for neon that $\kappa_1=-0.17$, $\kappa_2=0.18$, $\eta_{1,2}=-0.03$ leading to $\kappa=-0.02$. These results are in agreement with those of Ref. [2]. These cancellations take place on the amplitude level. There is a strong compensation between the contributions of the states with different values of j in the sums $\Sigma_j F_j^0 S_{j,i}$ in Eqs. (12) and (14). In other words, the correlations with different ns states compensate each other in the amplitude Eq. (12).

Thus in the case $\ell=1$, at least in the examples considered above, the IPA breaking effects appear to be rather large (of the order of about 20%), at intermediate energies which do not greatly exceed the binding energy of the K shell, since at these energies the correlations with the K shell are small [6]. However, at asymptotic energies the correlations with the K shell become large, canceling the total effect to a large extent. Ionization of a d electron of titanium ($Z=22$), considered in the nonrelativistic limit, is one more illustration of this tendency. Only the second terms of the rhs of Eqs. (14) and (15) contribute in the nonrelativistic approximation. Calculations carried out for $\omega=50$ keV give an IPA breaking effect of about 4%, while the individual contributions lead to magnitudes about ten times larger.

In the framework of our approach it is clear that such cancellations do not take place in ions with holes in s states, since the corresponding partial correlation becomes smaller if fewer electrons are available to participate in correlations. The lack of cancellations in ions was noted in Ref. [2].

The problem can also be studied experimentally. Investigation of the inverse process of radiative electron capture is more promising here. Capture by an ion is to be contrasted with capture by bare nuclei. In the latter case IPA is exact and there are no correlations—see Ref. [15] and references therein. Another interesting possibility is radiative capture to states with large values of ℓ.

In any event, due to the cancellations of the partial correlations for neutral ground-state atoms, the IPA breaking effects at energies of dozens of keV appear to be small, being of the order of relativistic corrections at these energies. This encourages performing relativistic analysis, which is, however of independent interest.

Now we wish to investigate the correlations for the relativistic case, when the ratio ω/m is no longer a small parameter. We may still start with the IPA amplitudes. The dependence of the amplitudes on the orbital momenta $F_{n\ell} \sim (\tau_{n\ell}/q)^\ell$ is still correct, but one cannot now neglect the photon momentum $\mathbf{k}$ in the transfer momentum $q=|\mathbf{p}-\mathbf{k}|$. Thus the connection between the amplitudes and the cross sections is not so simple as in the nonrelativistic case, requiring a complicated angular integration. Here, as a first step, we consider the asymptotic case $E \gg m$.

In this ultrarelativistic limit, the cross section is determined by momentum transferred to the nucleus $q \approx m$. Thus the energy dependence of the IPA cross sections in this limit is the same for all ℓ [4],

$$\sigma_{n\ell}^0(\omega) = \frac{\alpha(\alpha Z)^{2\ell+5}}{m\omega} c_{n\ell}, \quad (17)$$

with $c_{n\ell}$ coefficients of the order of unity, which do not depend on ω and αZ.

The corrections to this IPA equation are of the order of m/ω and of αZ. The energy dependence in Eq. (17) is the same for all ℓ, unlike in nonrelativistic IPA. The dependence on ℓ manifests itself in the factors $(\alpha Z)^{2\ell}$, which come from the normalization factors of the wave functions of the bound states.

It was shown in Ref. [12] that the relativistic amplitudes contain the Stobbe factor (SF), which is common for all the bound states and depends on the parameter $\pi\xi_Z$, if the terms of the order ξ_Z^2 are neglected. In the ultrarelativistic limit $\xi_Z = \alpha Z$. Due to the SF the leading corrections of the order $\pi\alpha Z$ to the rhs of Eq. (17) cancel in the cross-section ratios.

The IPA breaking corrections can be calculated by using Eq. (14). Recall that in the nonrelativistic limit the first term on the rhs of Eq. (14) is zero for even values of ℓ since the corresponding IPA amplitudes are purely real, if we use a conventional definition, in which the bound-state wave functions with $\ell_z = 0$ are real. The relativistic amplitudes contain both real and imaginary parts of the same order of magnitude for all values of ℓ. Neither part can be neglected without a more detailed analysis.

Including IPA breaking terms does not alter the common IPA dependence on the photon energy (for all ℓ), and employing Eq. (14) one rather obtains the corrections from the two terms of Eq. (8) as of the order

$$\frac{\sigma_{n\ell}(\omega) - \sigma_{n\ell}^0(\omega)}{\sigma_{n\ell}^0(\omega)} \sim \frac{\alpha}{(\alpha Z)^\ell}; \frac{\alpha^2}{(\alpha Z)^{2\ell}} \quad \text{for } \ell \geqslant 1, \quad (18)$$

with neglected terms of order $(\alpha Z)^2$. The magnitudes $\alpha/(\alpha Z)^\ell$ and $\alpha^2/(\alpha Z)^{2\ell}$, which follow from the analysis presented above, are the estimates of the first and second terms on the rhs of Eq. (14). The SFs, which are contained in the relativistic amplitudes beyond IPA (for the same reason as in the nonrelativistic case), cancel in the ratios (18).

For $\ell = 1$ the first term dominates if we assume $Z \gg 1$. In this case the IPA breaking effects are of the order $1/Z$. In the ionization of s states the correlations provide a small contribution of order α.

In the general relativistic case the IPA breaking correction to the square of the amplitude $|F_i|^2$ obtained by this approach is given by Eq. (14). The first and second terms contribute values of the order $\alpha/(\alpha Z)^\ell$ and $\alpha^2/(\alpha Z)^{2\ell}$ correspondingly. The second term is always positive. Thus for $\ell = 1$ the first term dominates, leading to a contribution of the order $1/Z$ as in Eq. (11). The second term provides a correction of the order $1/Z^2$. For higher values of ℓ one can not make a definite conclusion about the relative role of the two terms. The relative role of the second term with respect to the first one can be described by the parameter $\mu_\ell = (\alpha Z)^{1-\ell}/Z$. We find $\mu_2 = 0.31$ and $\mu_3 = 0.10$ for the lightest atoms containing d and f electrons, with the charges of the nuclei being 21 and 57, respectively. Thus as it stands now we do not see a situation in which the second term on the rhs of Eq. (14) can be neglected.

The strong cancellation of the partial contributions to the correlations seen in the nonrelativistic calculations makes taking relativistic effects into account increasingly important when comparing IPA and IPA breaking contributions. For example, the relativistic corrections appear to be important for the interplay of the correlations in the ionization of Ne and Ar at $\omega \sim 70$ keV, and at even smaller energies in the case of ionization of the d states of Ti. In these cases the relativistic corrections to the partial contributions to the correlations of the electrons from the different shells become of the order of the total correlation effect, calculated in the nonrelativistic approximation. It is not clear if the cancellations obtained in the nonrelativistic approximation still take place after taking account of relativistic effects.

We have traced the role of the IPA breaking effects in high-energy photoionization. In the ionization of states of light atoms with nonzero angular momentum, the correlations in the same (or more outer) subshells dominate until the energy well exceeds the binding energy of more inner shells. These IPA breaking contributions have now been detected in experiments. Inclusion of IPA breaking effects removes the discrepancy between the experimental data and theoretical predictions [1,6,8]. However, at energies greatly exceeding the binding energy of K electrons, the correlations involving different shells cancel to a large extent [2]. The total correlation effect at energies of dozens of keV appears to be of the same magnitude as the relativistic correlation corrections to the uncorrelated IPA amplitudes. Thus a full investigation of correlations, when comparing IPA and IPA breaking contributions, requires inclusion of relativistic effects. Investigation of correlations at relativistic energies of hundreds of keV is of independent interest, considering the complicated energy dependence of the relativistic IPA cross sections. In the ultrarelativistic limit the energy dependence for all the cross sections is the same, while correlations modify the αZ dependence, according to Eq. (18).

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